

Fig. 1

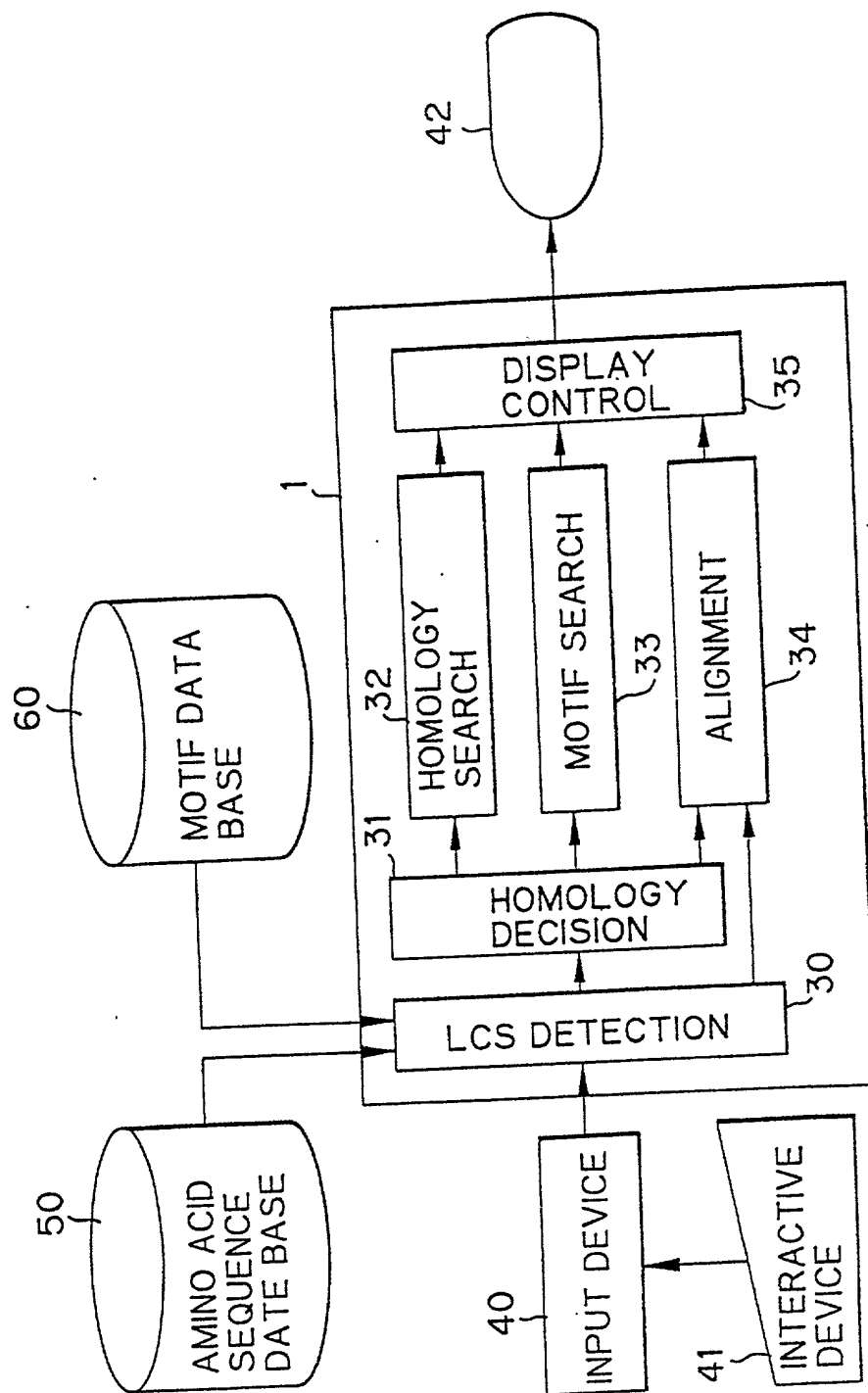


Fig. 2

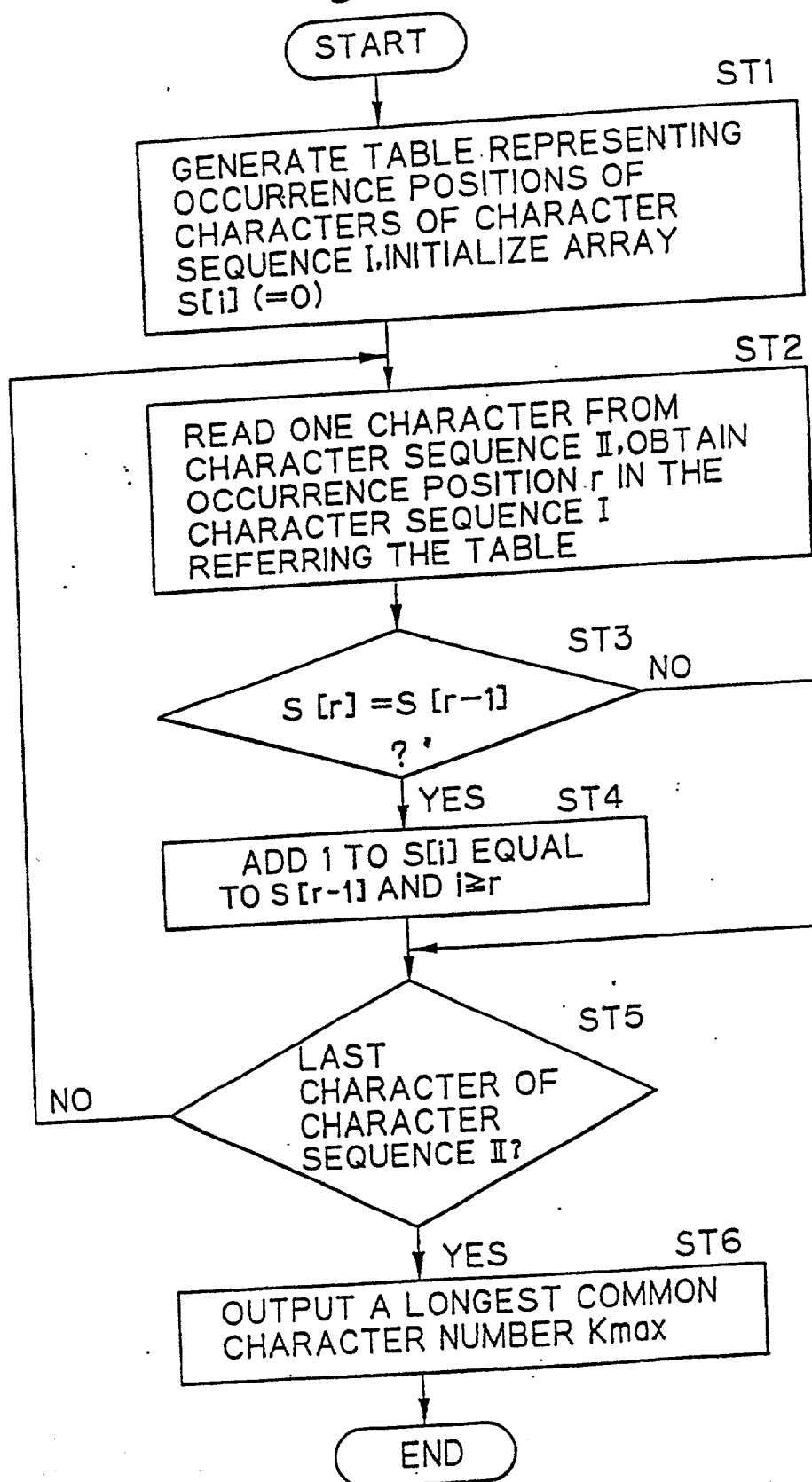


Fig. 3

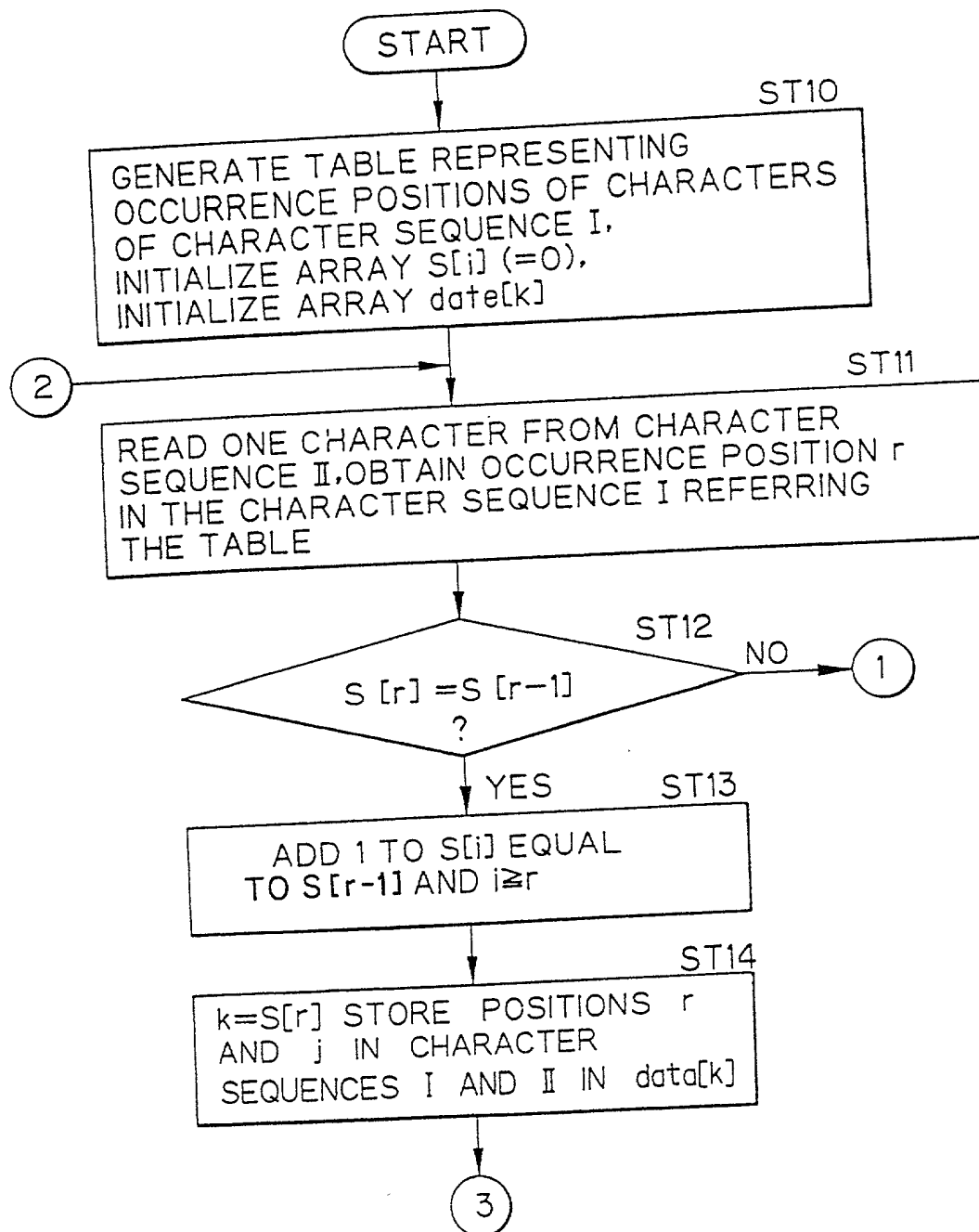


Fig. 4

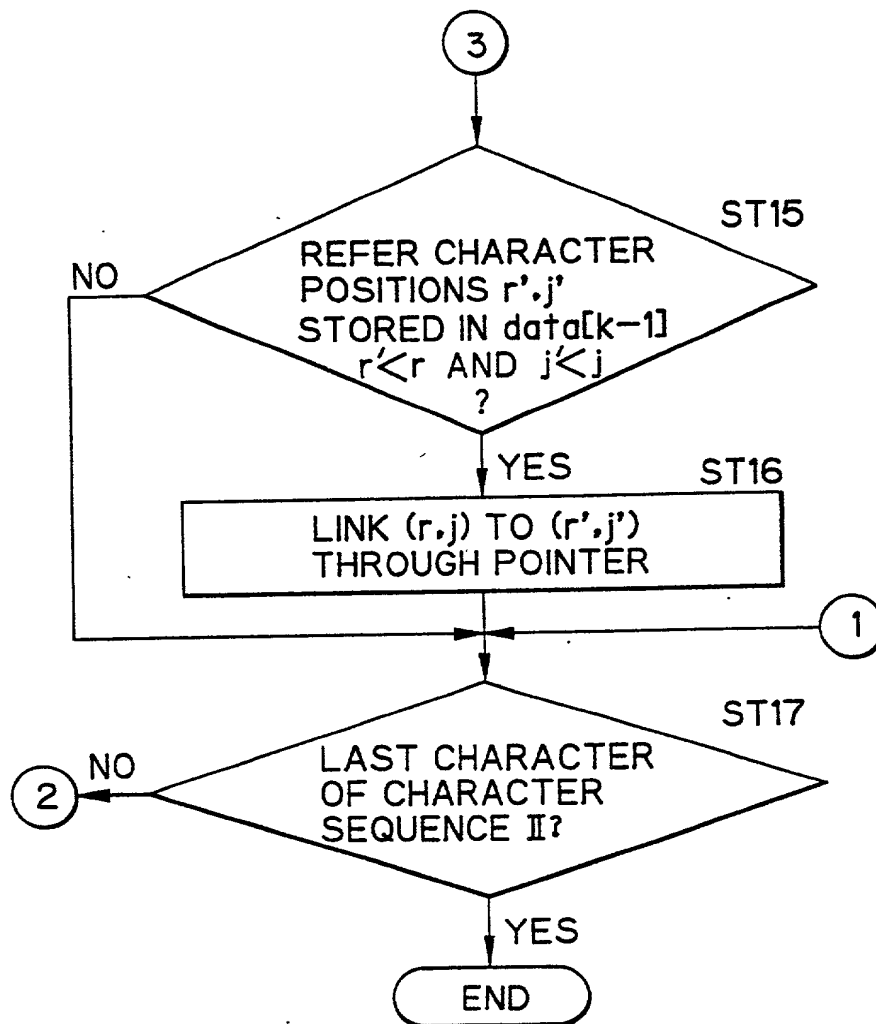


Fig. 5

CHARACTER SEQUENCE I="ABCB DAB"

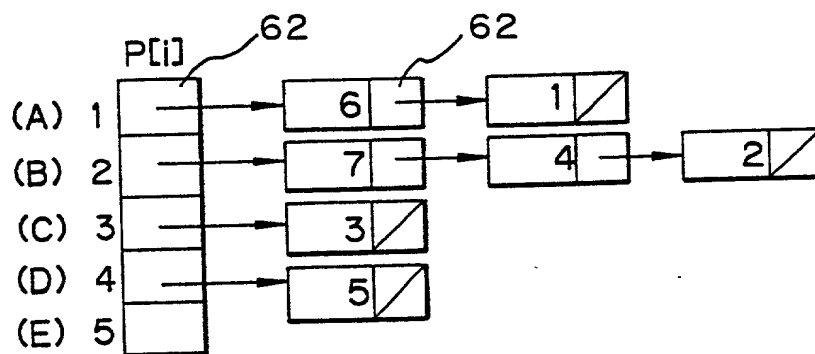


Fig. 6

CHARACTER SEQUENCE II = "BDCABA"

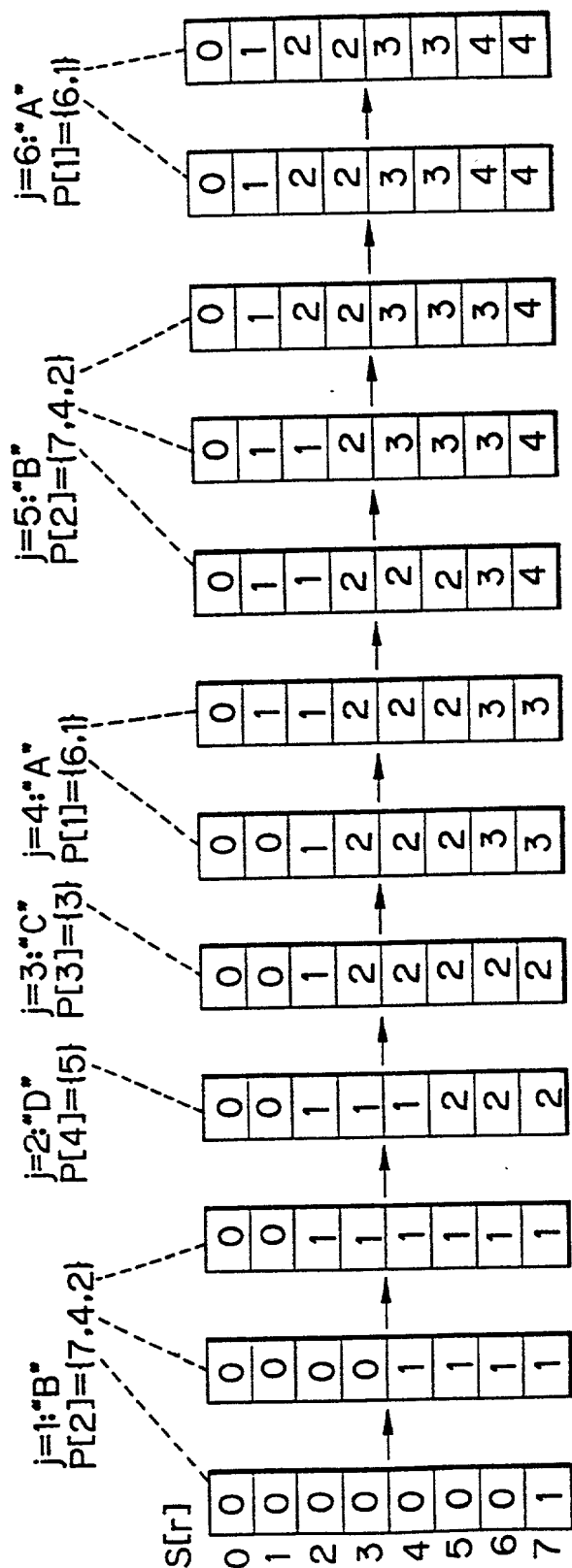


Fig. 7

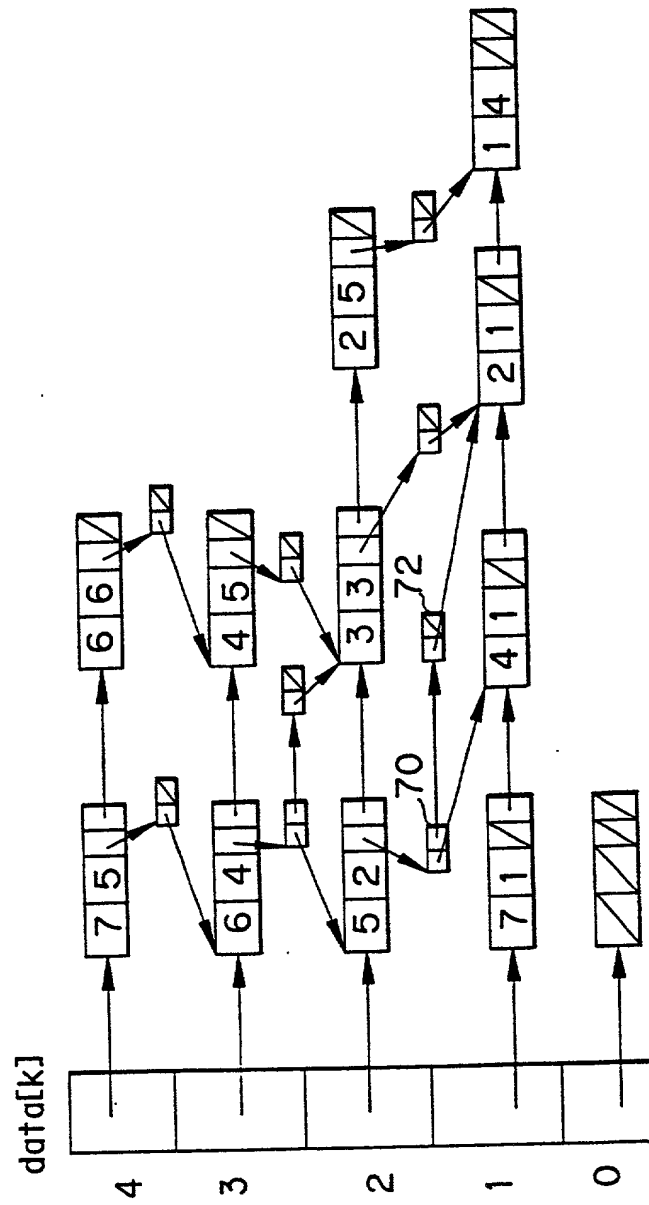


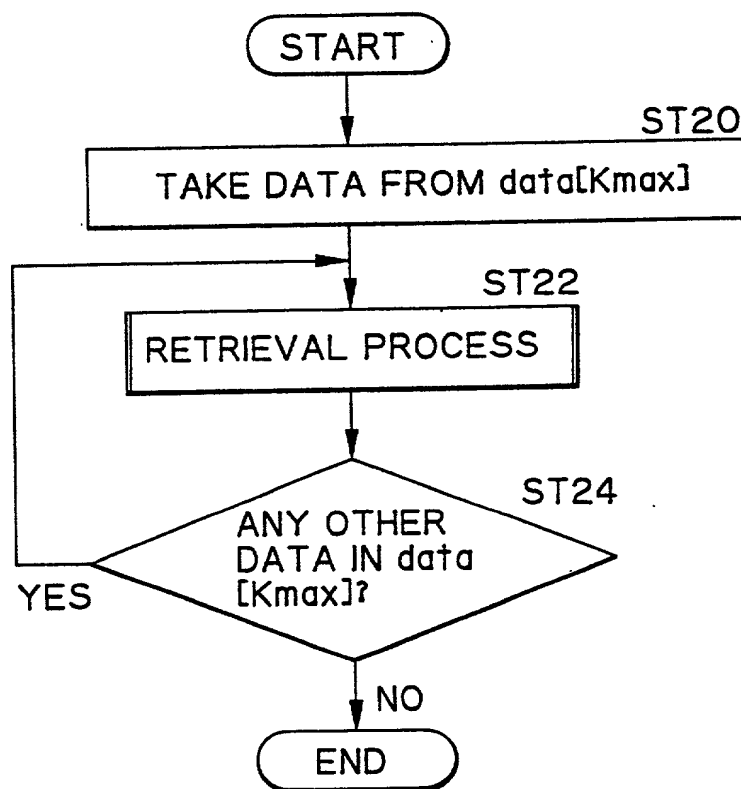
Fig. 8

Fig. 9

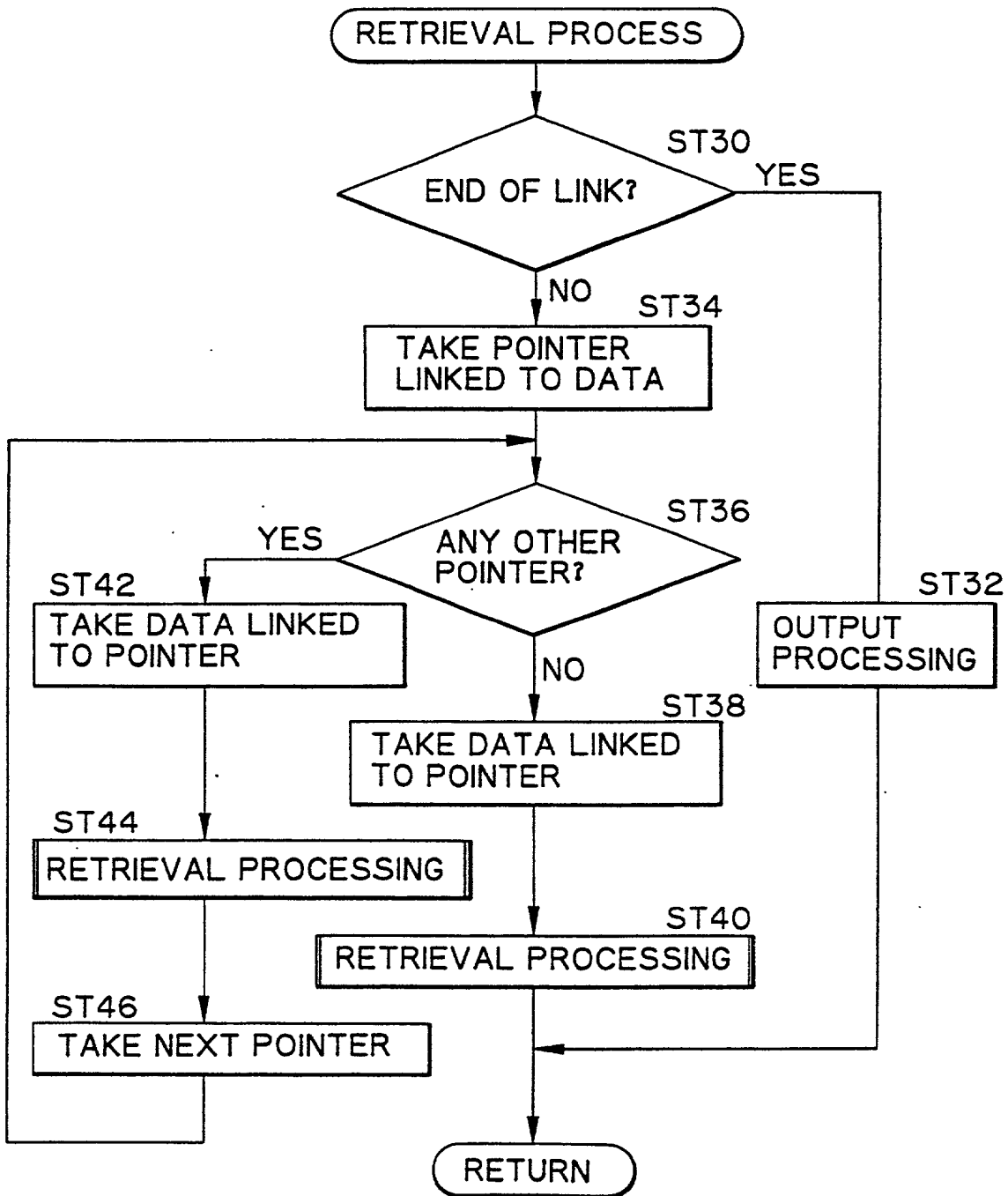


Fig. 10

human : GDVEKGKKIFIMKCSQCHTVEGGKHKTGPNLHGLFGRK
bacterium : EGDAAAGEKVSCKLACHTFDQGGANKVGPNPNLFGVF

LCS : GD{x3.3}G{x0.1}K{x0.2}K{x4.0}KC{x2.2}CHT{x3.3}GG{x2.2}K
GD{x1.4}E{x0.2}K{x0.2}K{x0.4}KC{x2.2}CHT{x3.3}GG{x2.2}K

homology : 47%

Rat : MSLAILRVIRLVRVFRIFKLSRHSKGLQILGRTLKASMRELGLLFFIGVV

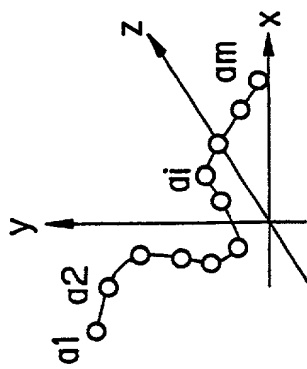
leucinzip. L{6}L{6}L{6}L{6}L

Fig. 11

Fig. 12

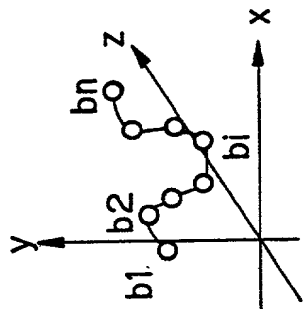
human : GDVEK G K KIFIMKCSQCHTVEKGG KHK TGP NLHGLFGRK ...
bacterium : E GDAAAGEK VSK KCLACHTFDQGGANKV GPNPN LFGVF...

Fig. 13 A



$$A = \{a_1, a_2, \dots, a_i, \dots, a_m\}$$

Fig. 13 B



$$B = \{b_1, b_2, \dots, b_j, \dots, b_n\}$$

Fig. 13 C

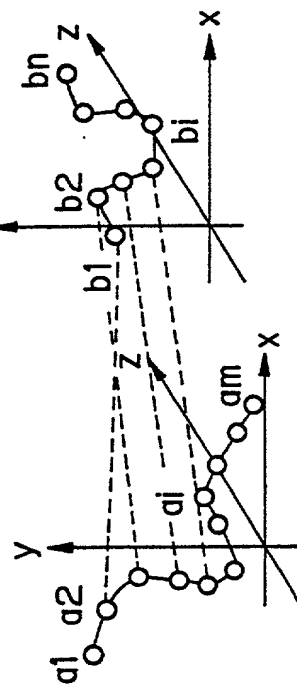


Fig. 13 D

$$r.m.s.d = \frac{\sqrt{\sum_{k=1}^n w_k (U b_k - a_k)^2}}{n}$$



Fig. 15

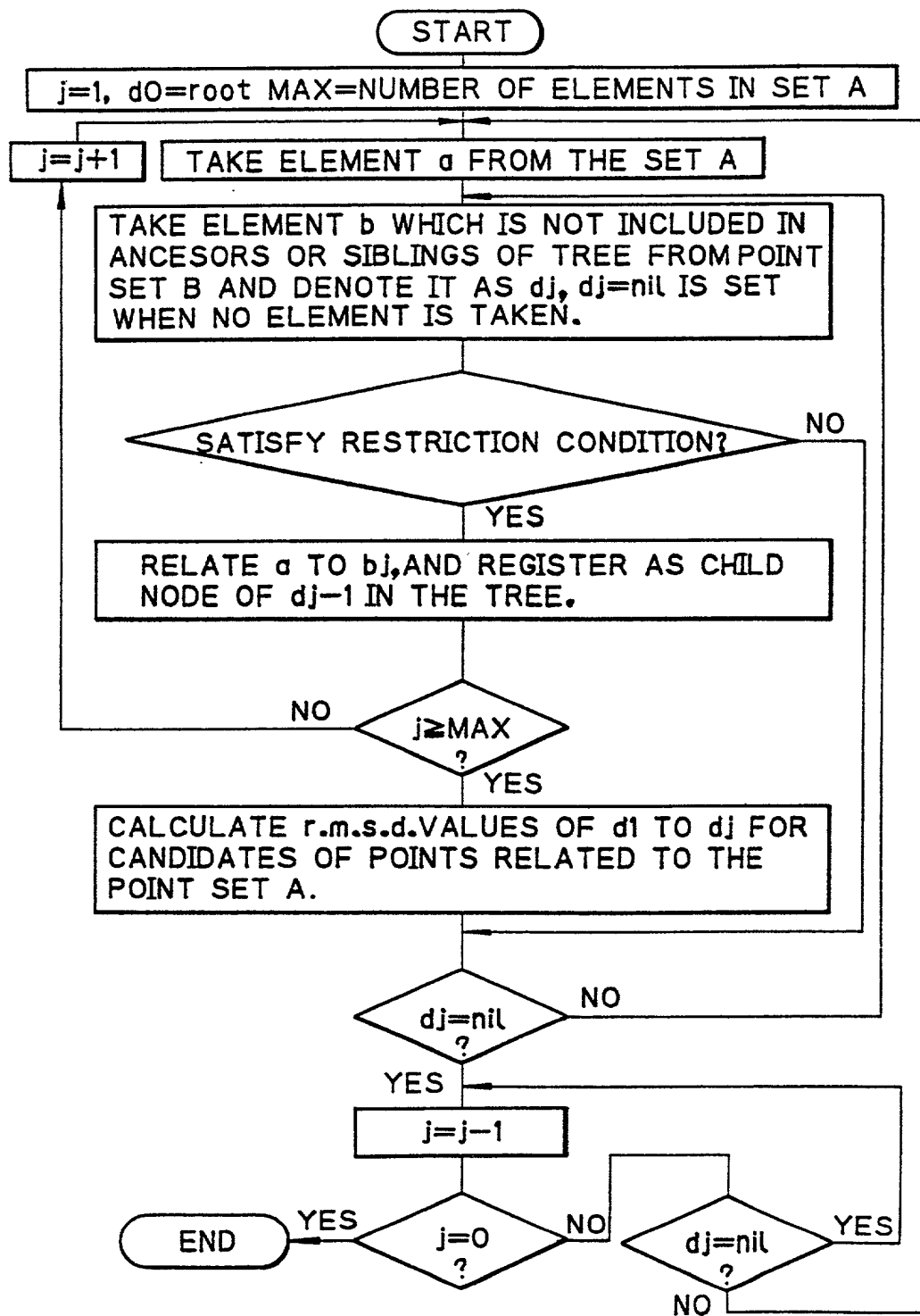


Fig. 14 A

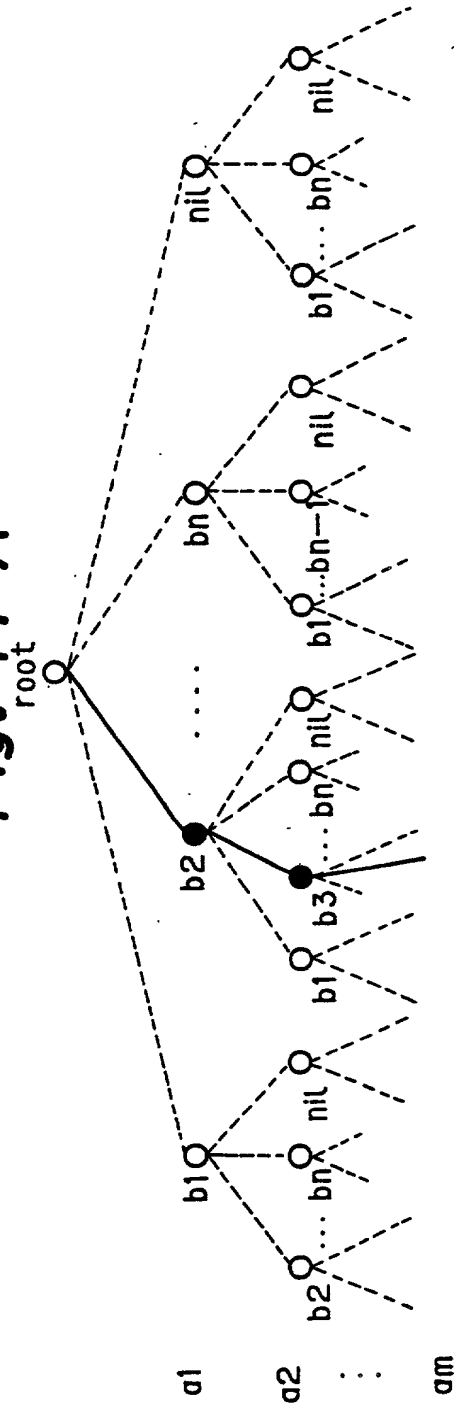


Fig. 14 B

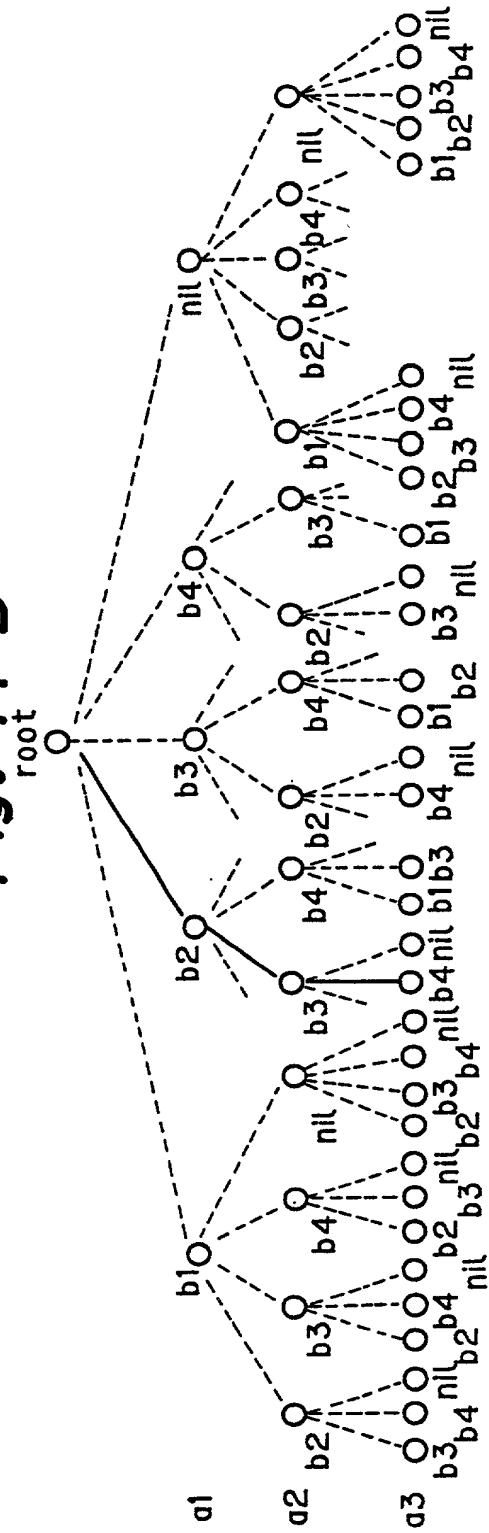


Fig. 17

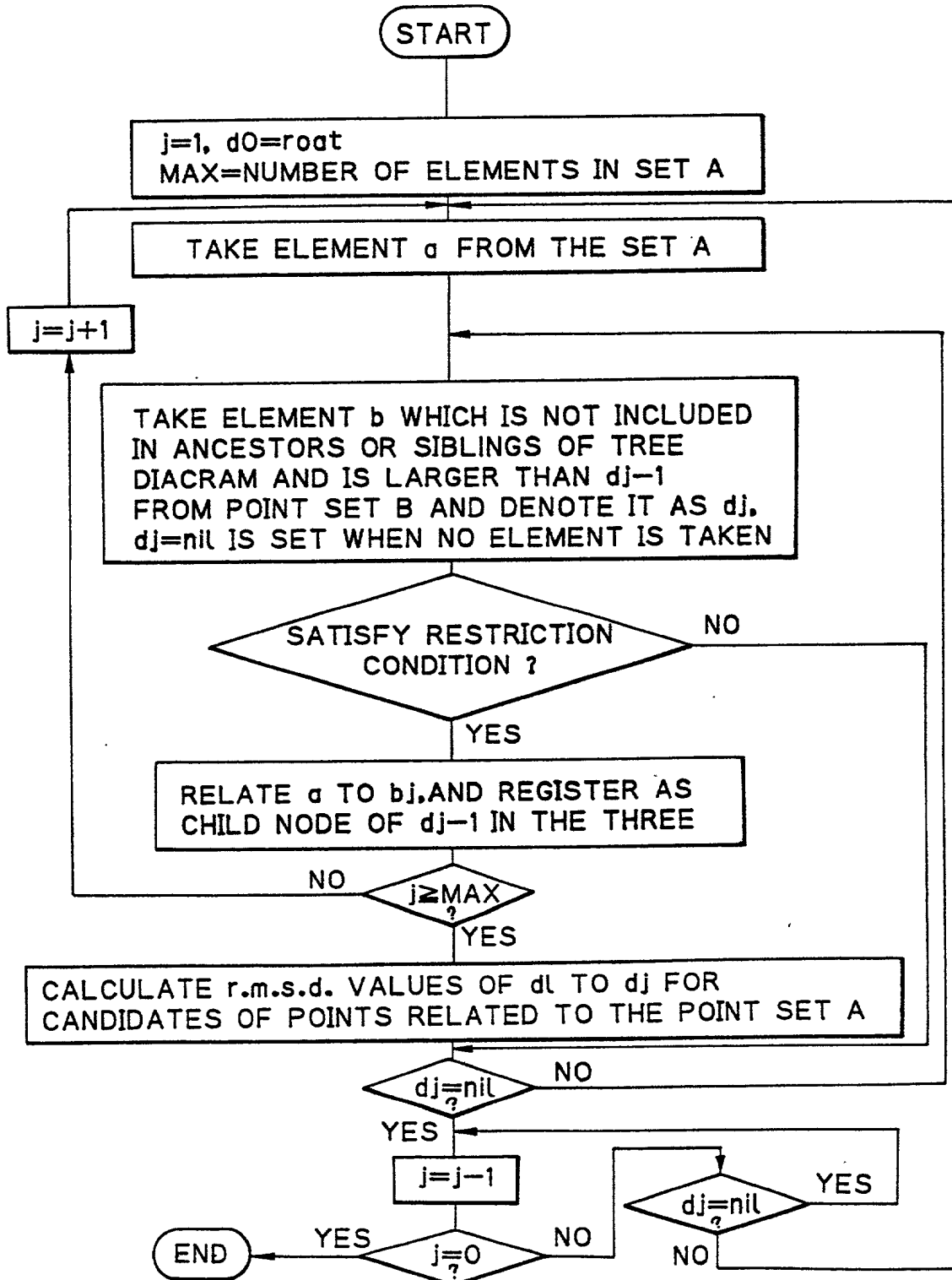


Fig. 19 A

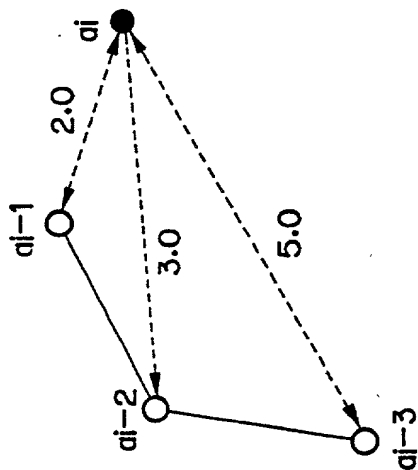


Fig. 19 B

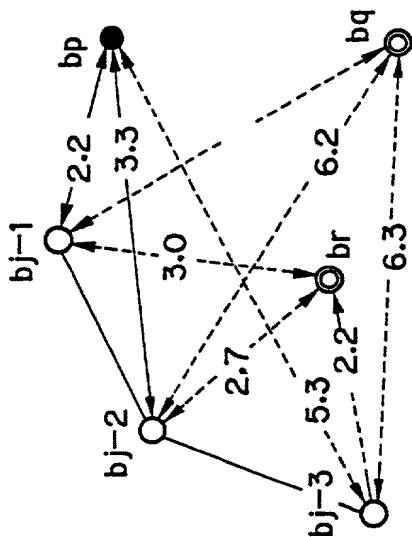


Fig. 20 A

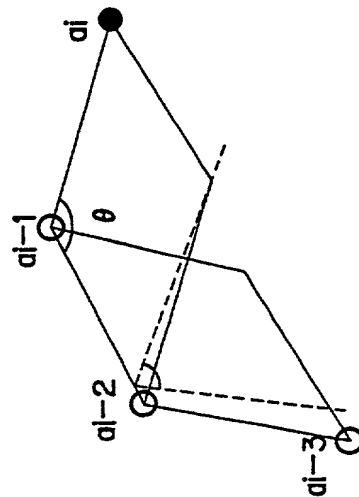


Fig. 20 B

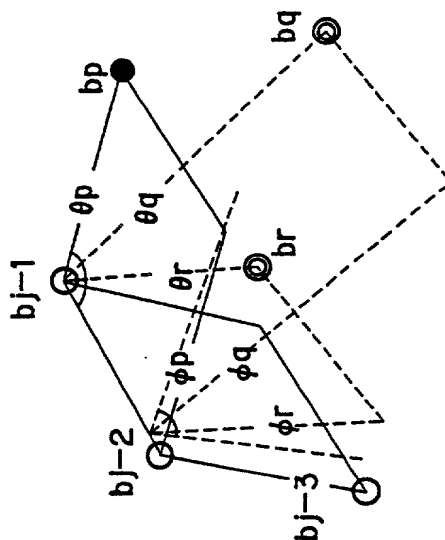


Fig. 21

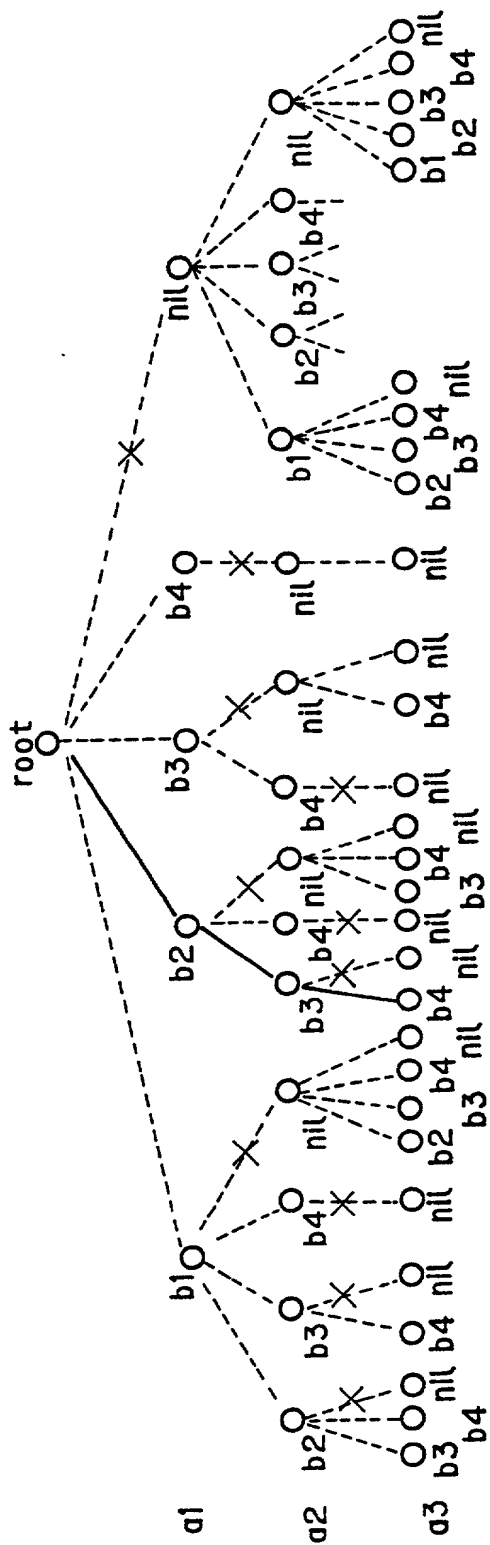


Fig. 22

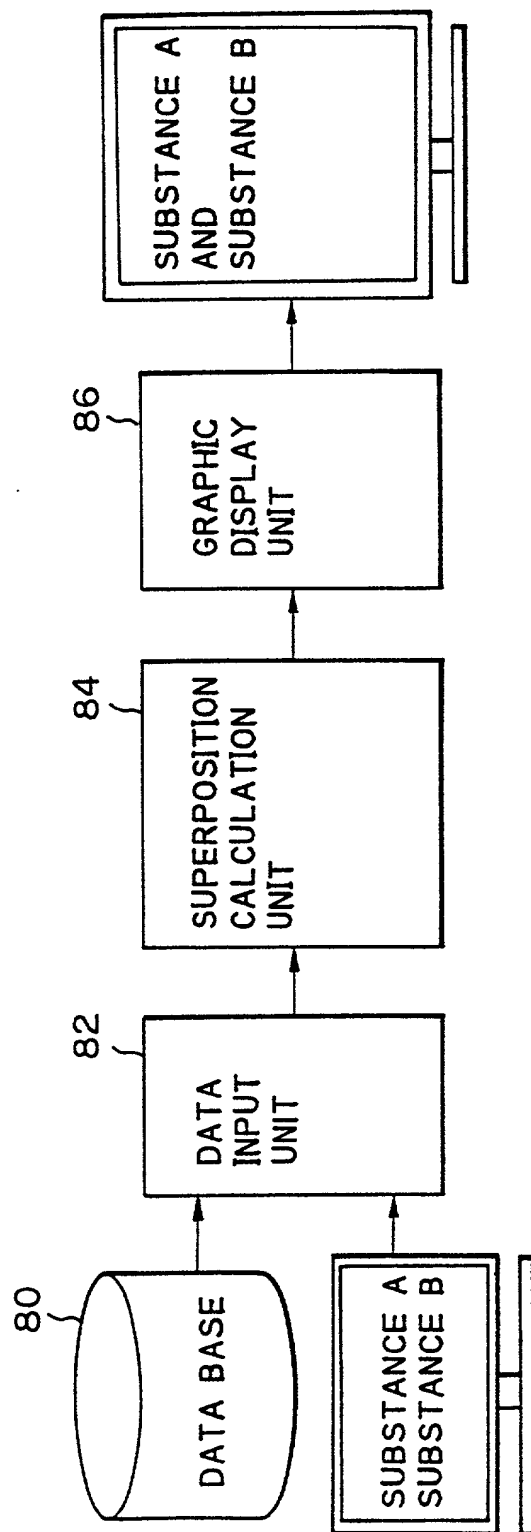


Fig. 23 B

AMINO ACID SEQUENCE OF CALMODULIN
(EXCERPT FROM PDB)

AMINO ACID SEQUENCE OF TROPONIN C
(EXCERPT FROM PDB)

Fig. 24 A

CALMODULIN

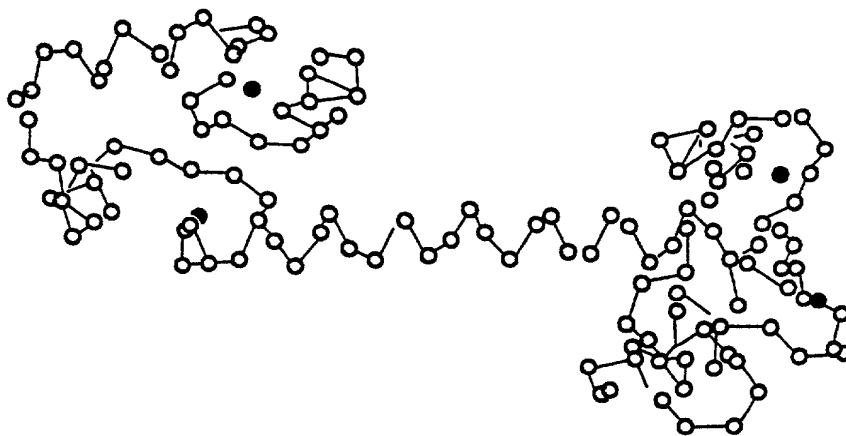


Fig. 24 B

TROPONIN C

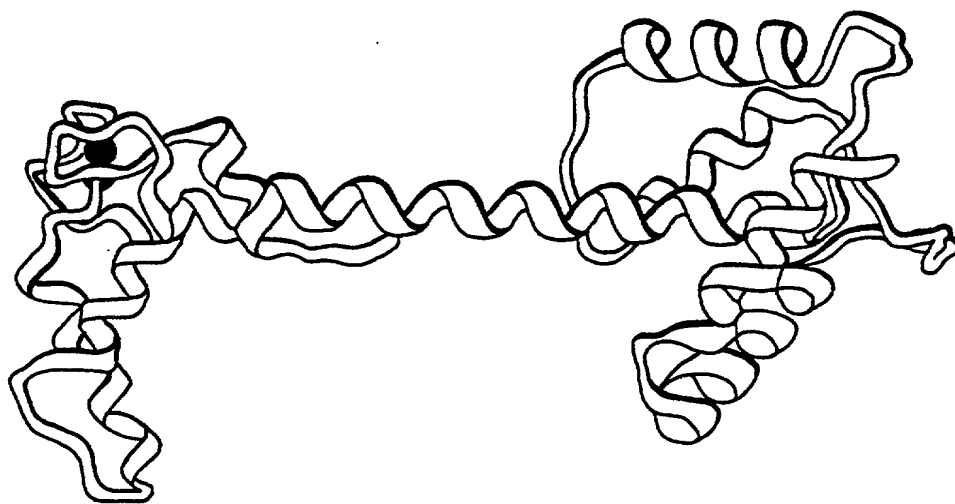


Fig. 25

Probe site = 81-108 in Calmodulin

| | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------------|------------|
| 96 | 97 | 98 | 99 | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | |
| L | A | D | C | F | R | I | F | D | K | N | A | D | G | F | < target > |
| I | R | E | A | F | R | V | F | D | K | D | G | N | G | Y | < probe > |
| 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120 | 121 | 122 | 123 | | | |
| I | D | I | E | E | E | L | G | E | I | L | R | A | T | < target > | |
| I | S | A | A | E | E | L | R | H | V | M | T | N | L | < probe > | |

rmsd = 0.567034

Fig. 26

Probe site = 81-108 and 117-143 in Calmodulin

| | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----------|----------|----------|---|--|
| 96 | 97 | 98 | 99 | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | | | |
| L | A | D | C | F | R | I | F | D | K | N | A | D | G | F | < target | > | |
| I | R | E | A | F | R | V | F | D | K | D | G | N | G | Y | < probe | > | |
| 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120 | 121 | 122 | 123 | | | | | |
| I | D | I | E | E | L | G | E | I | L | R | A | T | < target | > | | | |
| I | S | A | A | E | L | R | H | V | M | T | N | L | < probe | > | | | |
| 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 | 141 | 142 | 143 | 144 | 145 | | | | |
| I | E | D | L | M | K | D | S | D | K | N | N | D | G | < target | > | | |
| V | D | E | M | I | R | E | A | N | I | D | G | D | G | < probe | > | | |
| 146 | 147 | 148 | 149 | 150 | 151 | 152 | 153 | 154 | 155 | 156 | 157 | 158 | | | | | |
| R | I | D | F | D | E | F | L | K | M | M | E | G | < target | > | | | |
| Q | V | N | Y | E | E | F | V | Q | M | M | T | A | < probe | > | | | |

rmsd = 0.823665

Fig. 27

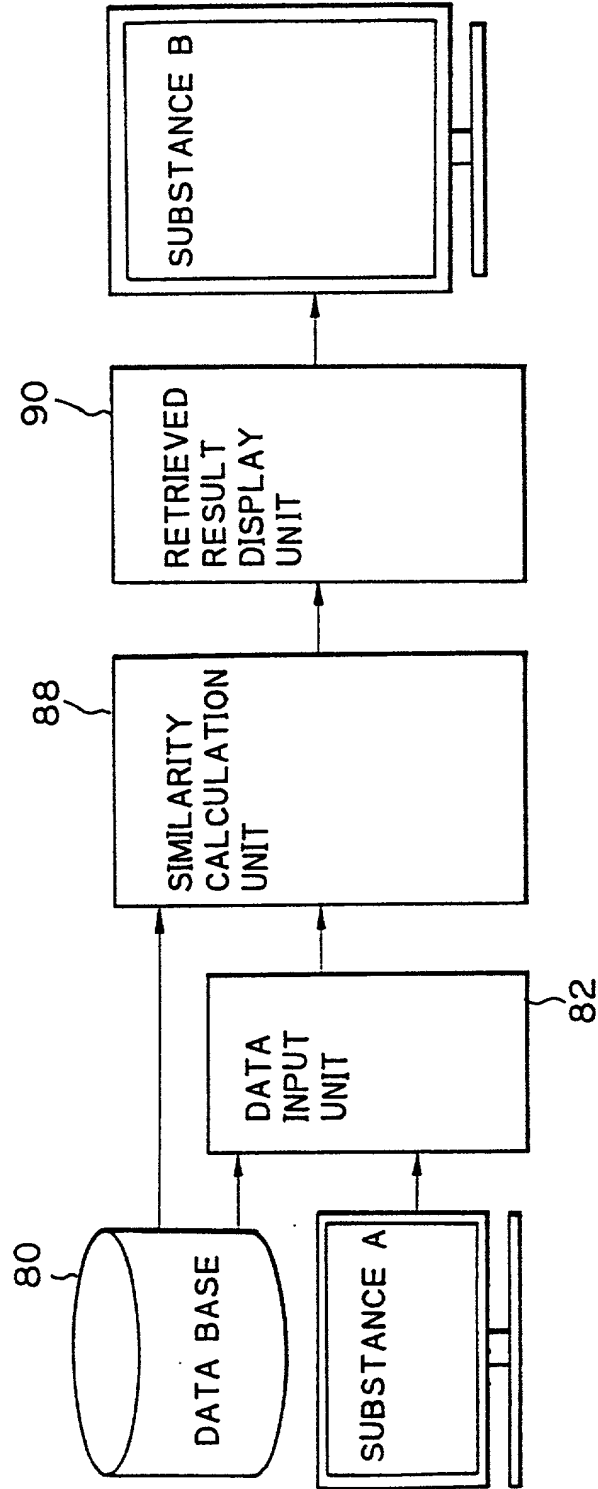


Fig. 28

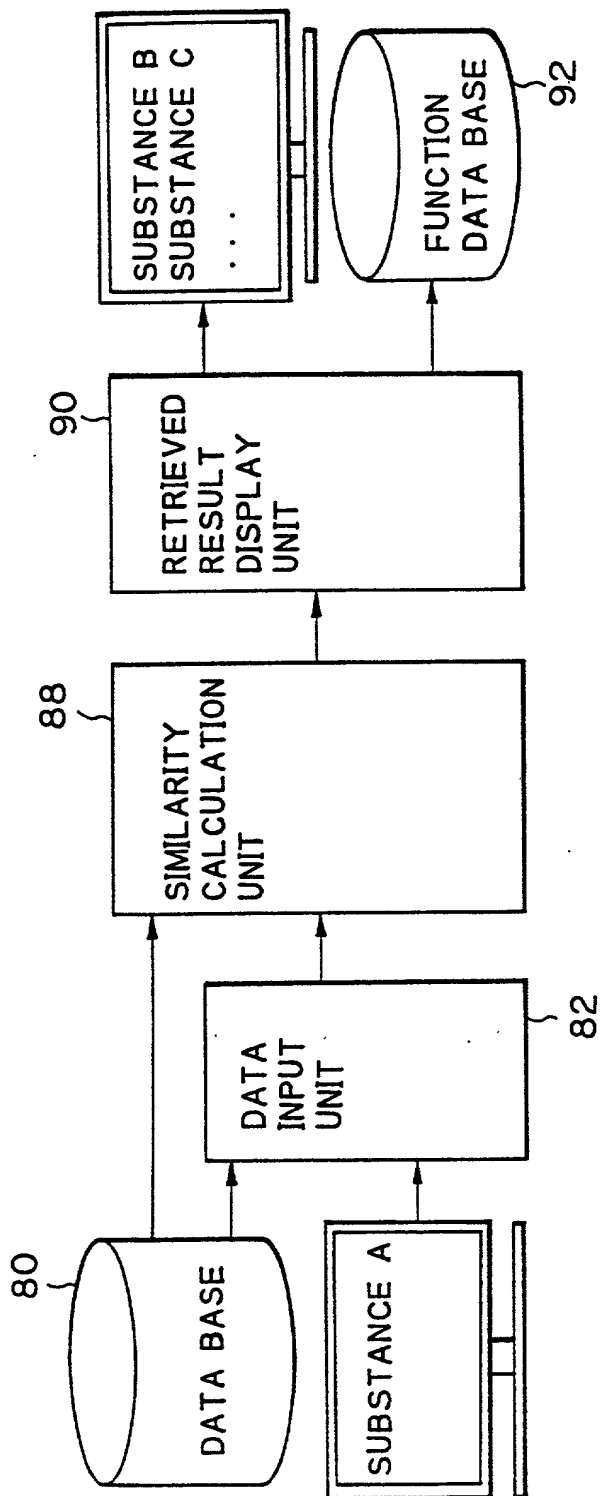


Fig. 29

===== ATP/GTP binding site =====

Probe = (elongation factor)

7 8 9 10 11 12 13 14
G H V D H G K T < probe >

8 9 10 11 12 13 14 15
G A P G S G K G < target >
G H V D H G K T < probe >
rmsd=0.648732 adenylate kinase

unit - A

: : :
: : :
: : :
10 11 12 13 14 15 16 17
G A G G V G K S < target >
G H V D H G K T < probe >
rmsd=0.421770 ras protein

Fig. 30

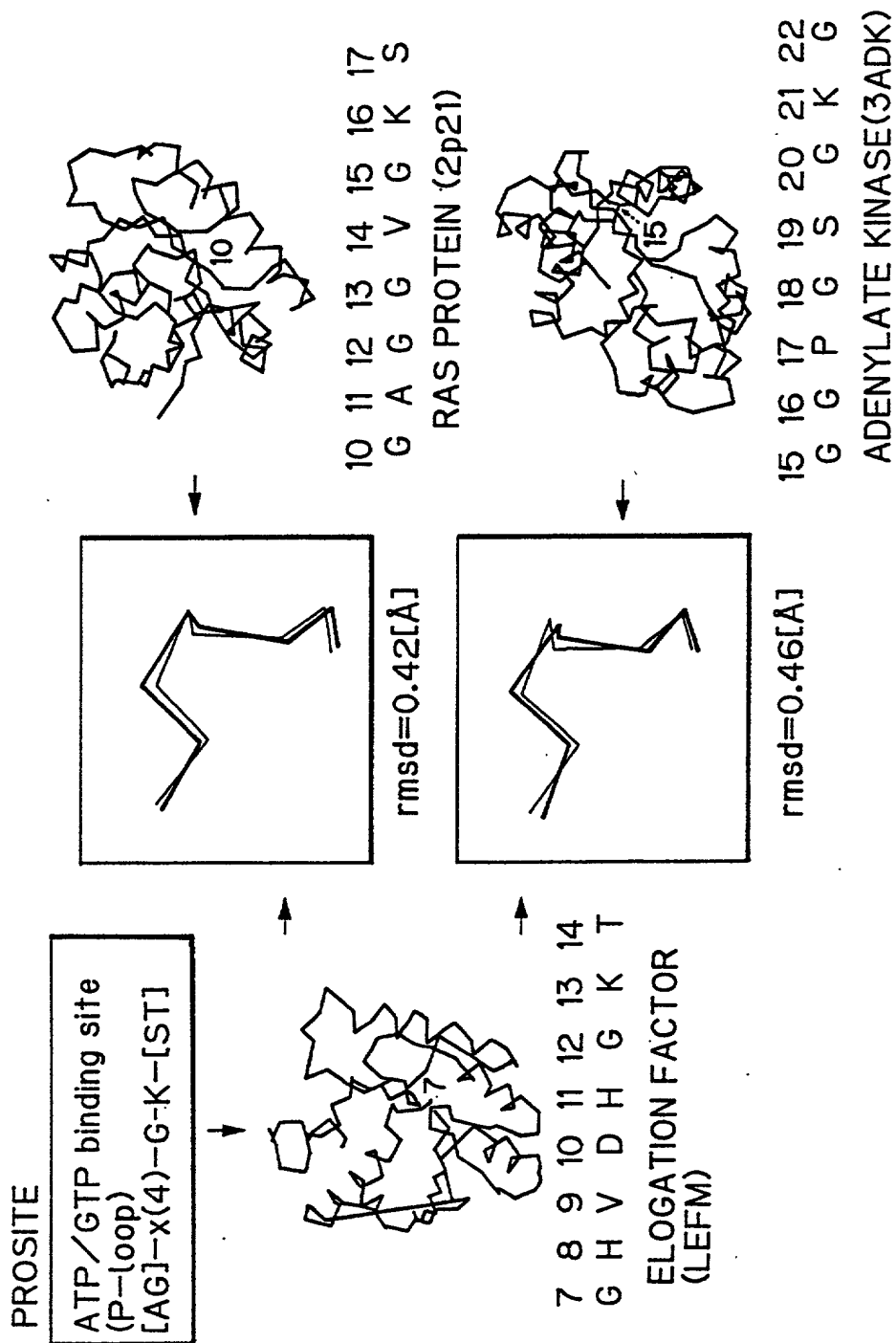


Fig. 31

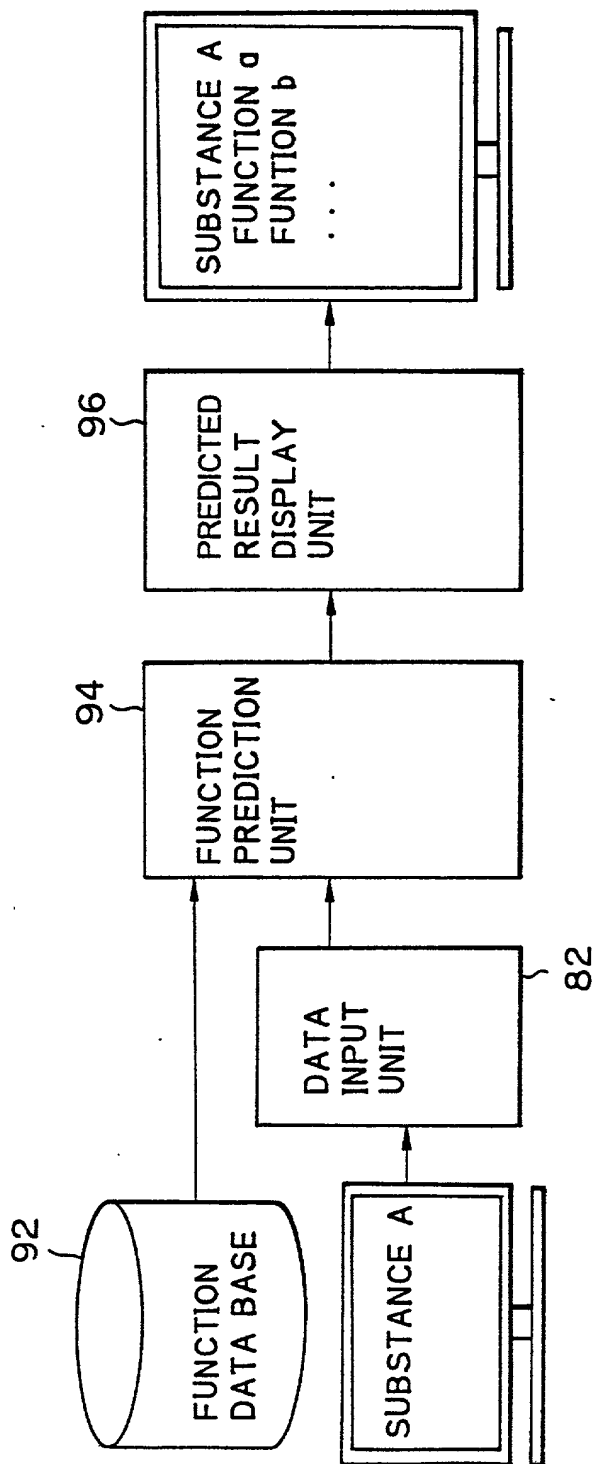


Fig. 32 B

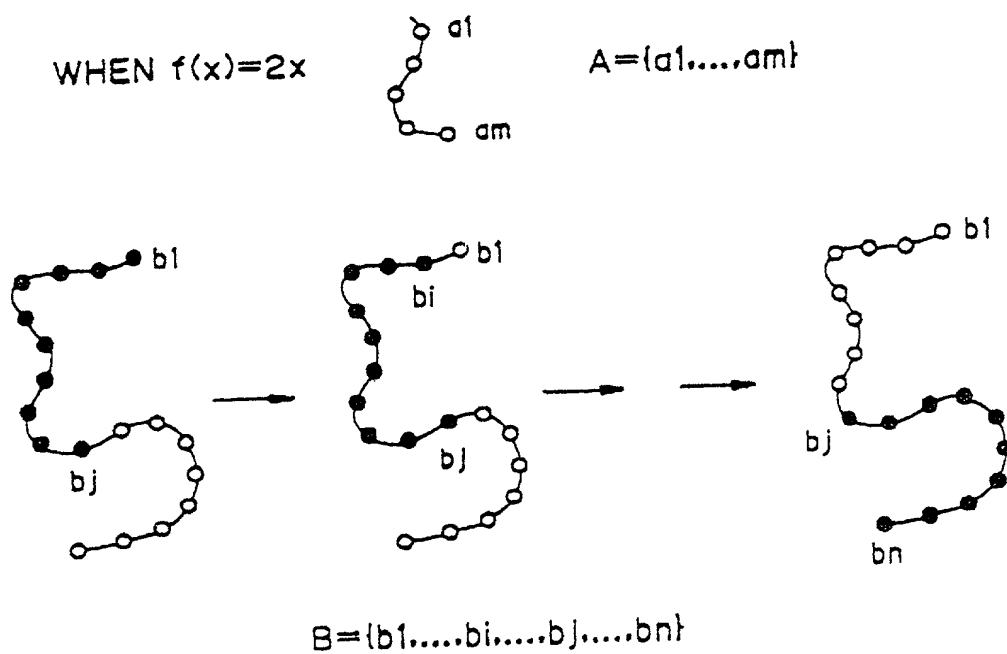
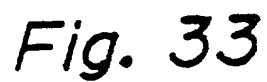


Fig. 34

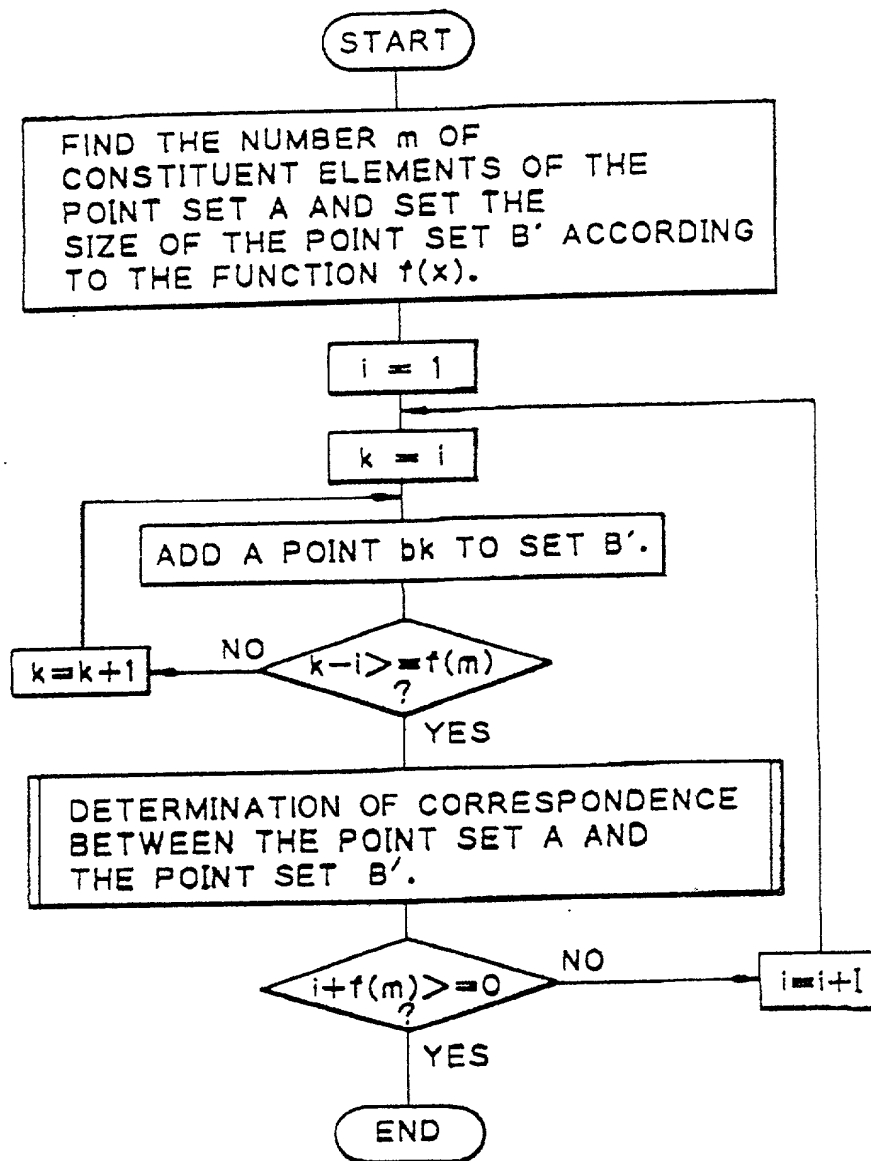
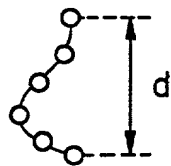
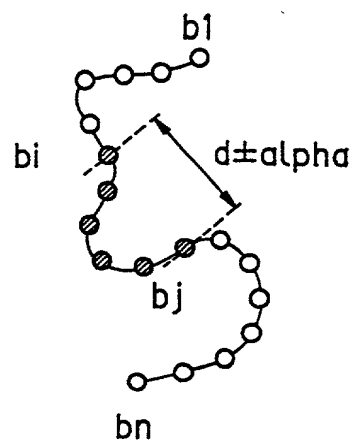


Fig. 35 A



$$A = \{a_1, a_2, \dots, a_m\}$$

Fig. 35 B



$$B = \{b_1, \dots, b_i, \dots, b_j, \dots, b_n\}$$

Fig. 36

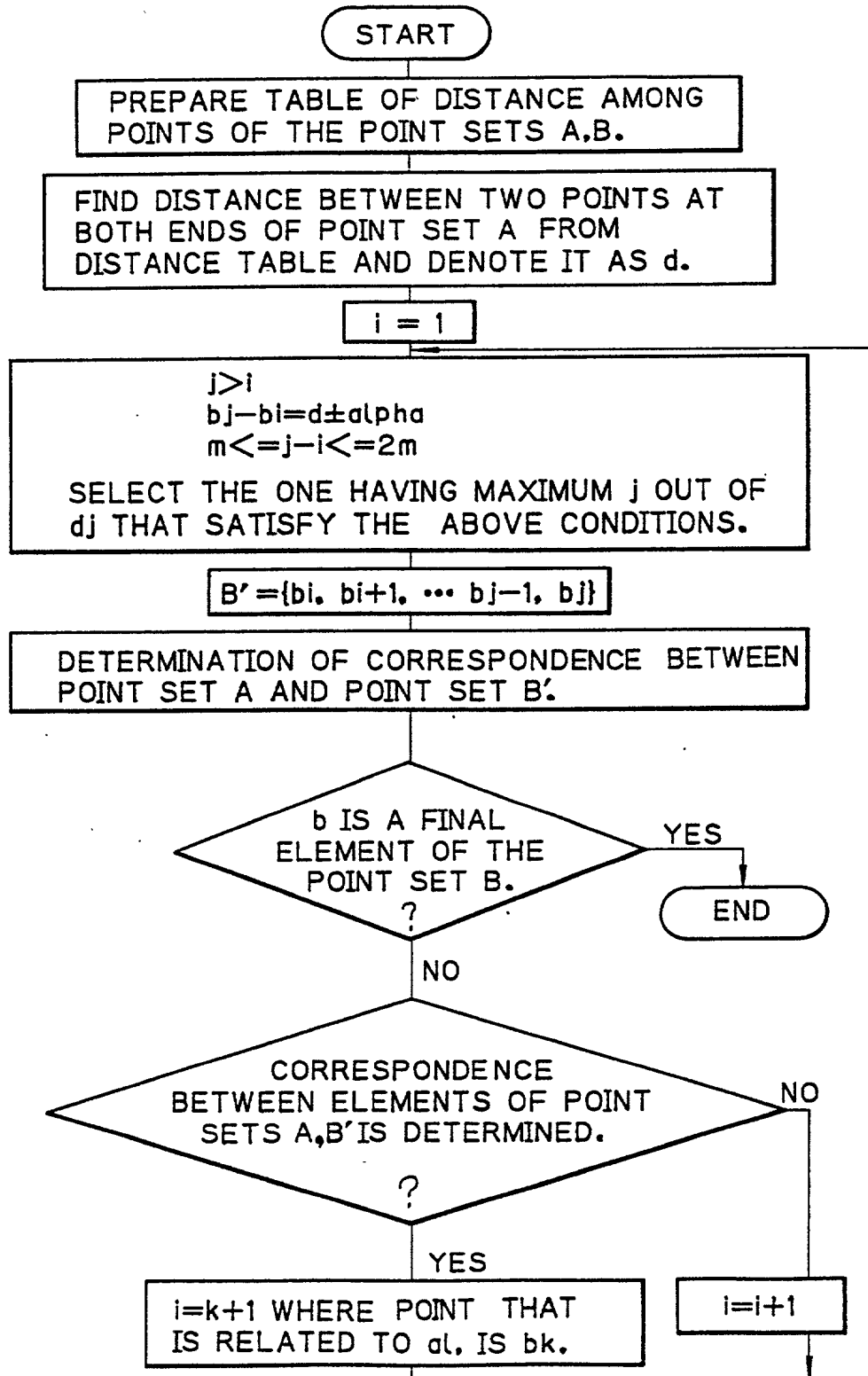


Fig. 37.

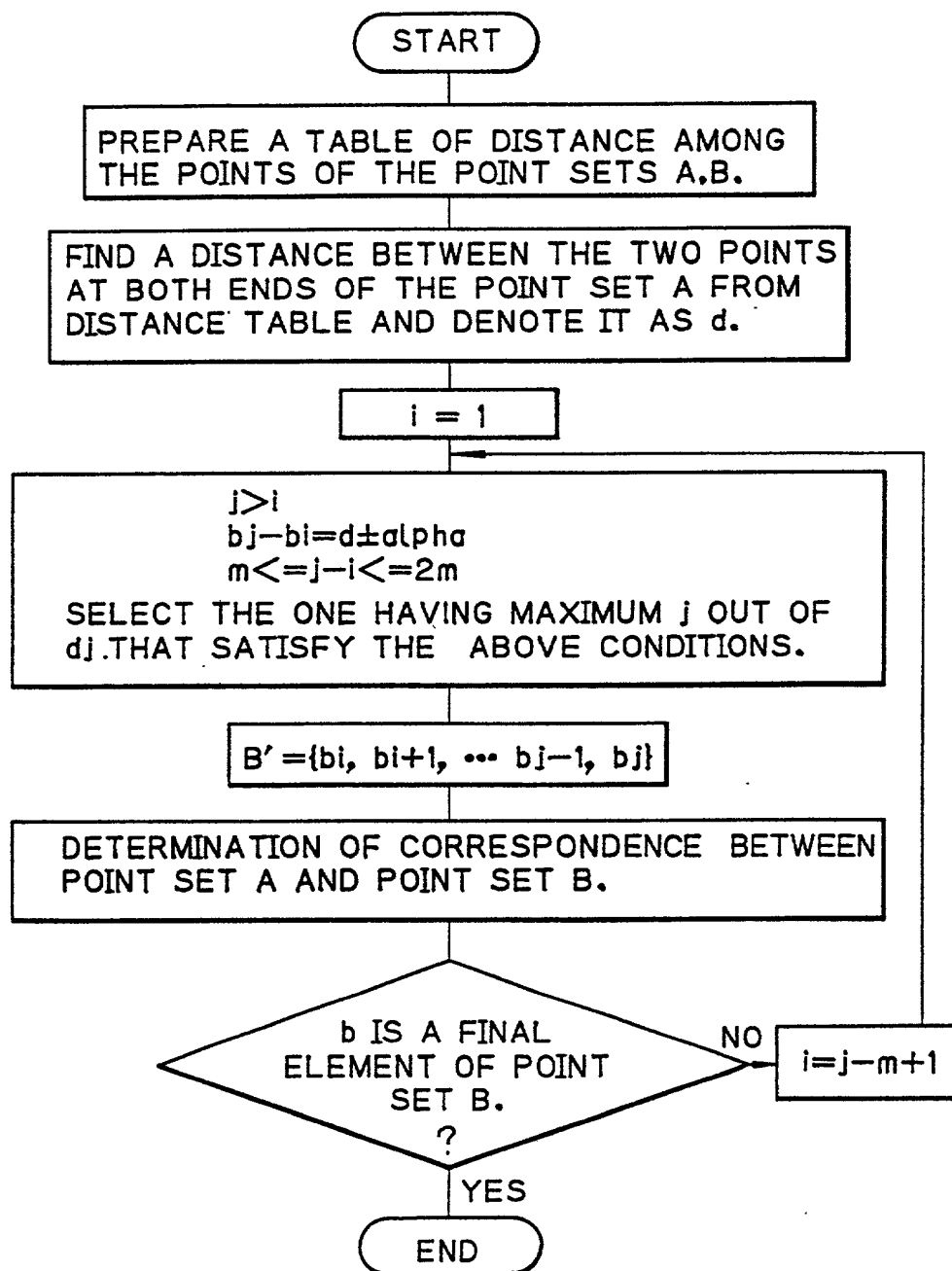


Fig. 38 A

| | | | | | | | | | | | | | | | | | | | | |
|-----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | I | V | G | G | Y | T | C | C | A | N | T | V | P | Y | Q | V | S | L | N | S |
| 21 | G | Y | H | F | C | G | G | S | L | I | N | S | Q | W | V | V | S | A | A | H |
| 41 | C | Y | K | S | G | I | Q | V | R | L | G | E | D | N | I | N | V | V | E | G |
| 61 | N | E | Q | F | I | S | A | S | K | S | I | V | H | P | S | Y | N | S | N | T |
| 81 | L | N | N | D | I | M | L | I | K | L | K | S | A | A | S | L | N | S | R | V |
| 101 | A | S | I | S | L | P | T | S | C | A | S | A | G | T | Q | C | L | I | S | G |
| 121 | W | G | N | T | K | S | S | G | T | S | Y | P | D | V | L | K | C | L | K | A |
| 141 | P | I | L | S | D | S | S | C | K | S | A | Y | P | G | Q | I | T | S | N | M |
| 161 | F | C | A | G | Y | L | E | G | G | K | D | S | C | Q | G | D | S | G | G | P |
| 181 | V | V | C | S | G | K | L | Q | G | I | V | S | W | G | S | G | C | A | Q | K |
| 201 | N | K | P | G | V | Y | T | K | V | C | N | Y | V | S | W | I | K | Q | T | I |
| 221 | A | S | N | | | | | | | | | | | | | | | | | |

AMINO ACID SEQUENCE OF TRYPSIN (EXCERPT FROM PDB)

Fig. 38 B

| | | | | | | | | | | | | | | | | | | | | |
|-----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | V | V | G | G | T | E | A | Q | R | N | S | W | P | S | Q | I | S | L | Q | Y |
| 21 | R | S | G | S | S | W | A | H | T | C | G | G | T | L | I | R | Q | N | W | V |
| 41 | M | T | A | A | H | C | V | D | R | E | L | T | F | R | V | V | V | G | E | H |
| 61 | N | L | N | Q | N | N | G | T | E | Q | Y | V | G | V | Q | K | I | V | V | |
| 81 | P | Y | W | N | T | D | D | V | A | A | G | Y | D | I | A | L | L | R | L | A |
| 101 | Q | S | V | T | L | N | S | Y | V | Q | L | G | V | L | P | R | A | G | T | I |
| 121 | L | A | N | S | P | C | Y | I | T | T | G | W | G | L | T | R | T | N | G | Q |
| 141 | L | A | Q | T | L | Q | Q | A | Y | L | P | T | V | D | Y | A | I | C | S | S |
| 161 | S | S | Y | W | G | S | T | V | K | N | S | M | V | C | A | G | G | D | G | V |
| 181 | R | S | G | C | Q | G | D | S | G | G | P | L | H | C | L | V | N | G | Q | Y |
| 201 | A | V | H | G | V | T | S | F | V | S | R | L | G | C | N | V | T | R | K | P |
| 221 | T | V | F | T | R | V | S | A | Y | I | S | W | I | N | N | V | I | A | S | N |

AMINO ACID SEQUENCE OF ELASTASE (EXCERPT FROM PDB)

Fig. 39 A

Key site number 36 – 41 in Trypsin

| | | | | | | | |
|----|----|----|----|----|----|------------|--|
| 41 | 42 | 43 | 44 | 45 | 46 | | |
| M | T | A | A | H | C | < target > | |
| V | S | A | A | H | C | < probe > | |

d = 12.070038 [A]

r.m.s.d. = 0.061077 [A]

The number of atoms in a probe = 6

The number of atoms in PDB = 240

The number of combination = 1

Time = 1sec

RETRIEVED RESULTS OF HISTIDINE ACTIVE SITES

Fig. 39 B

Key site number 175 – 179 in Trypsin

| | | | | | | |
|-----|-----|-----|-----|-----|------------|--|
| 186 | 187 | 188 | 189 | 190 | | |
| G | D | S | G | G | < target > | |
| G | D | S | G | G | < probe > | |

d = 8.922721 [A]

r.m.s.d. = 0.092879 [A]

The number of atoms in a probe = 5

The number of atoms in PDB = 240

The number of combination = 1

Time = 1sec

RETRIEVED RESULTS OF SERINE ACTIVE SITES

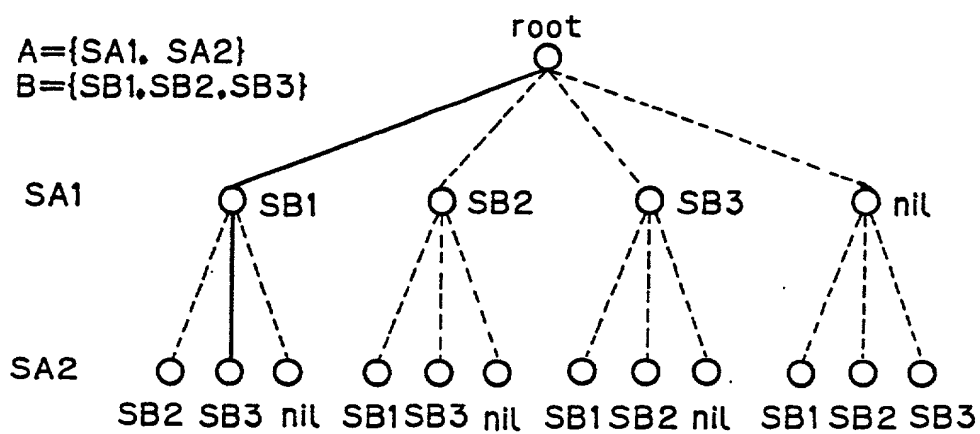
Fig. 40

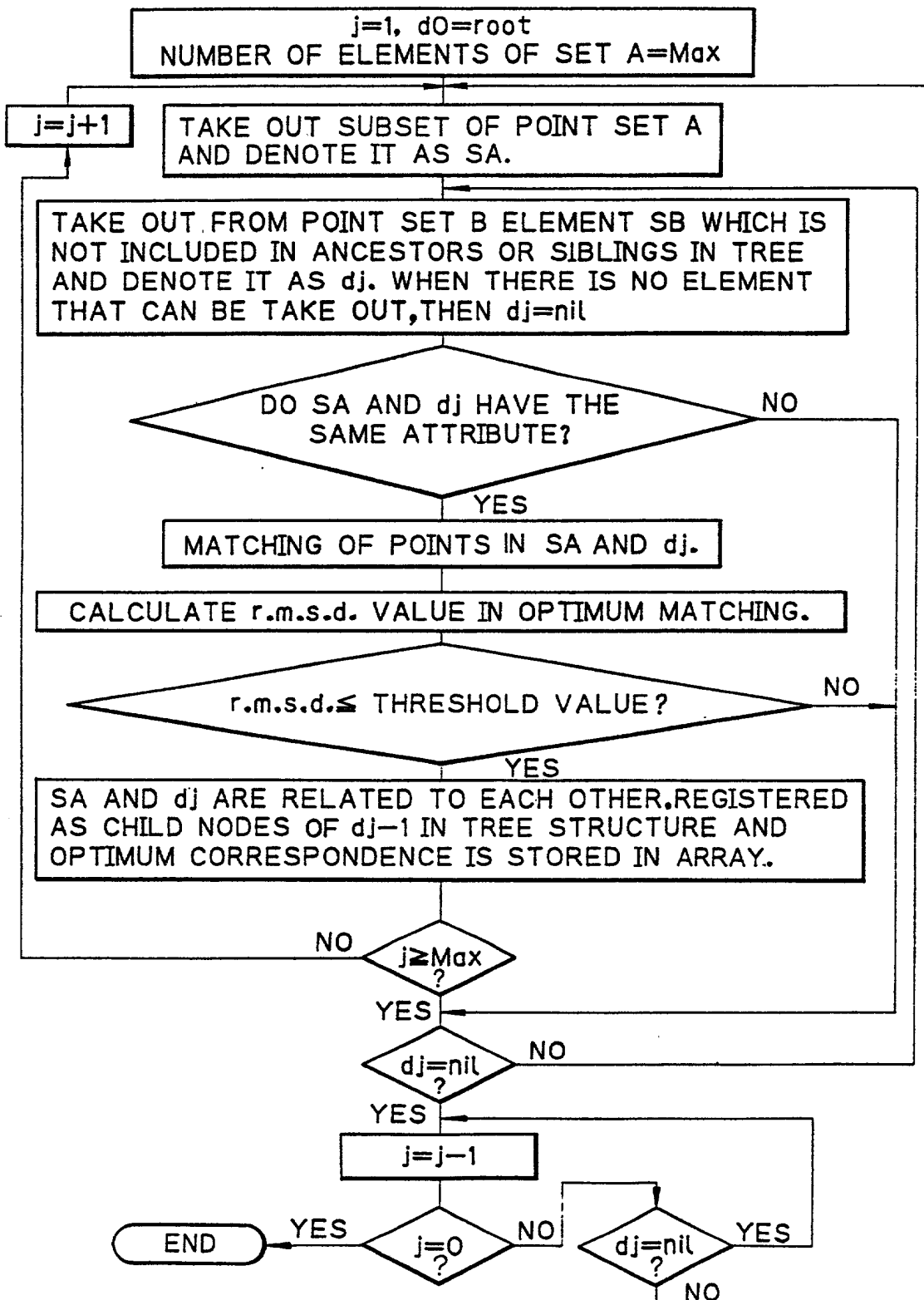
Fig. 41

Fig. 42

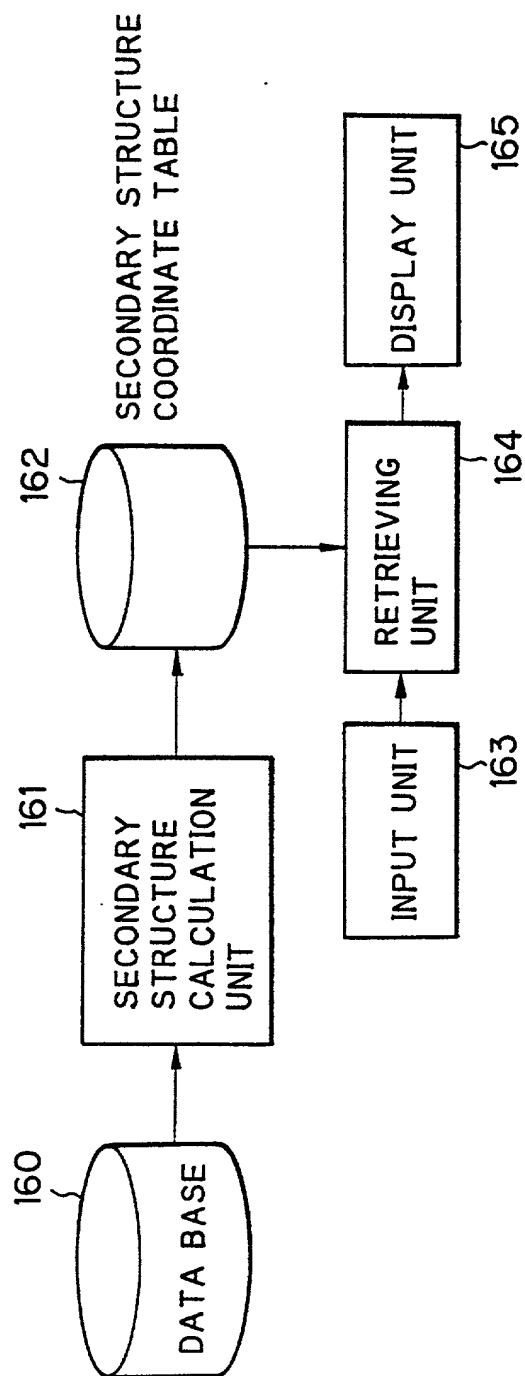


Fig. 43

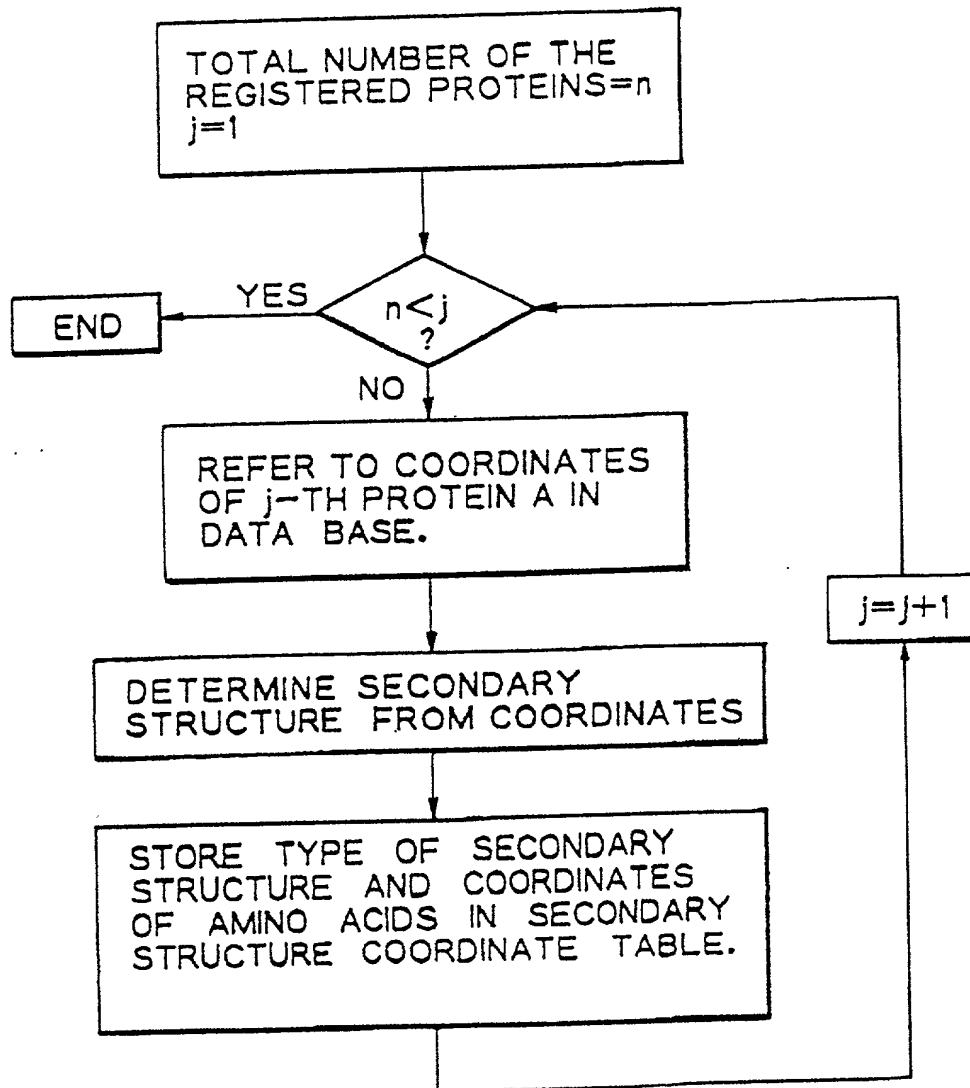


Fig. 44

162

| SUBSET | COORDINATES | TYPE |
|----------------|--------------------------------------|------------------|
| S1 | $\{X_1, X_2, X_3, X_4, \dots, X_a\}$ | α - HELIX |
| S2 | $\{X_{a+1}, X_{a+2}, \dots, X_b\}$ | α - HELIX |
| S3 | $\{X_{b+1}, X_{b+2}, \dots, X_c\}$ | β - SHEET |
| S4 | $\{X_{c+1}, X_{c+2}, \dots, X_d\}$ | β - SHEET |
| | \vdots | \vdots |
| S _n | $\{X_{l+1}, X_{l+2}, \dots, X_m\}$ | 3 - TURN |

Fig. 45

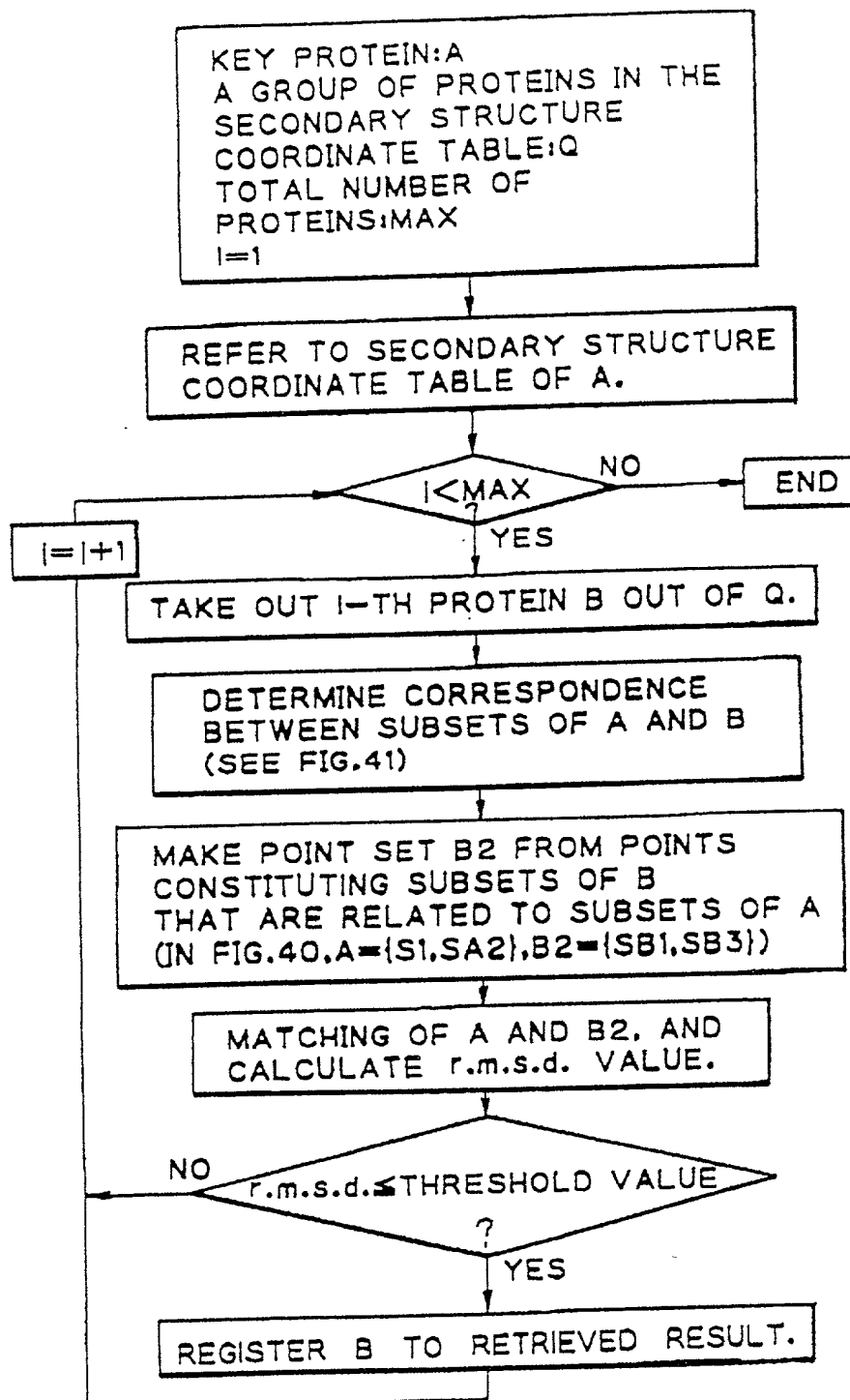


Fig. 46

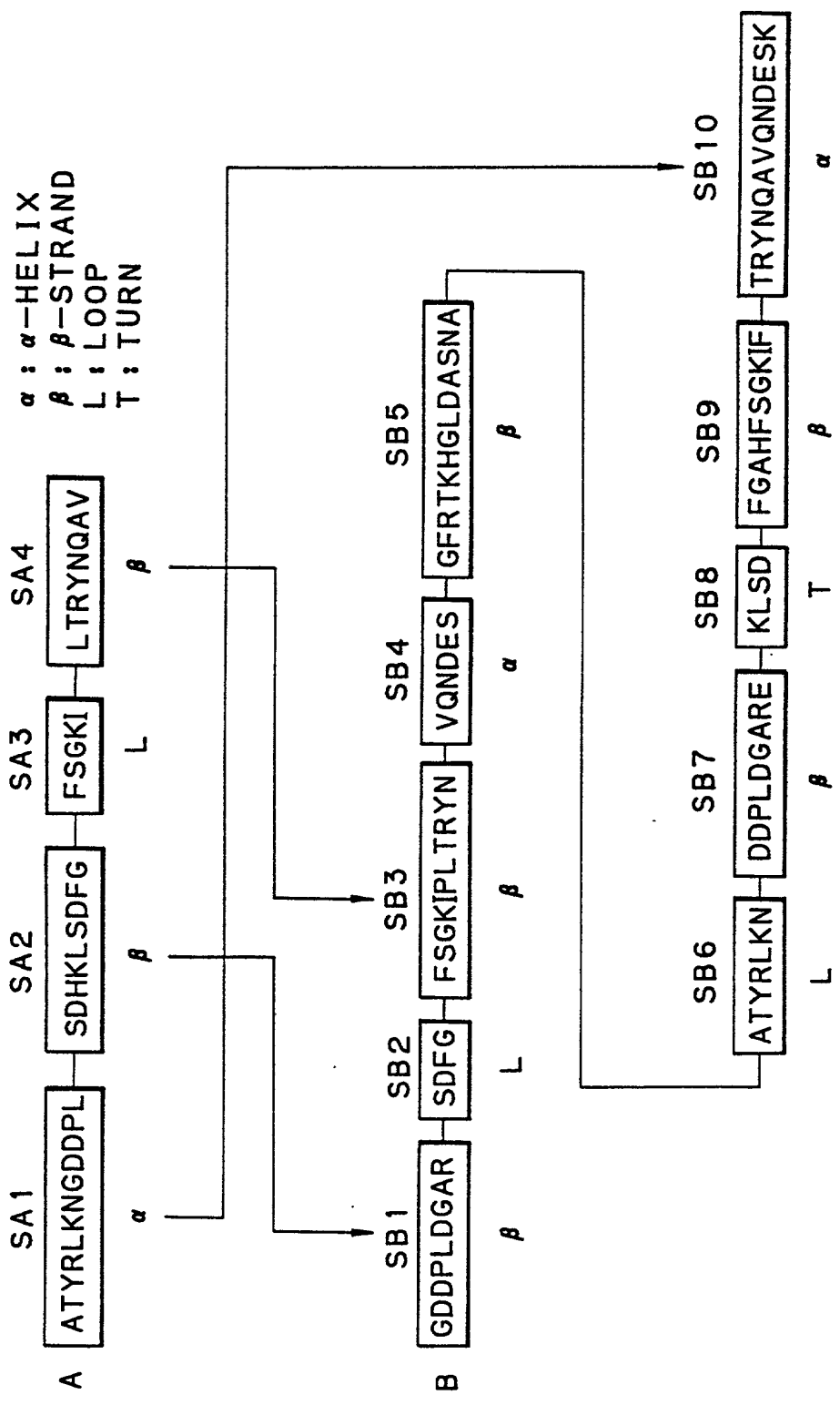
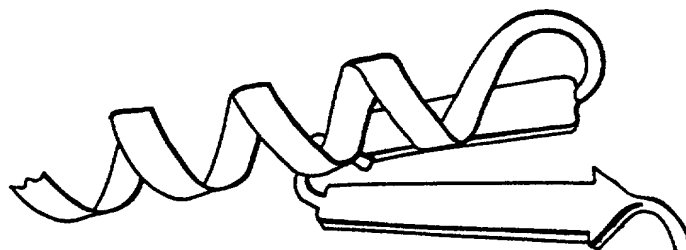
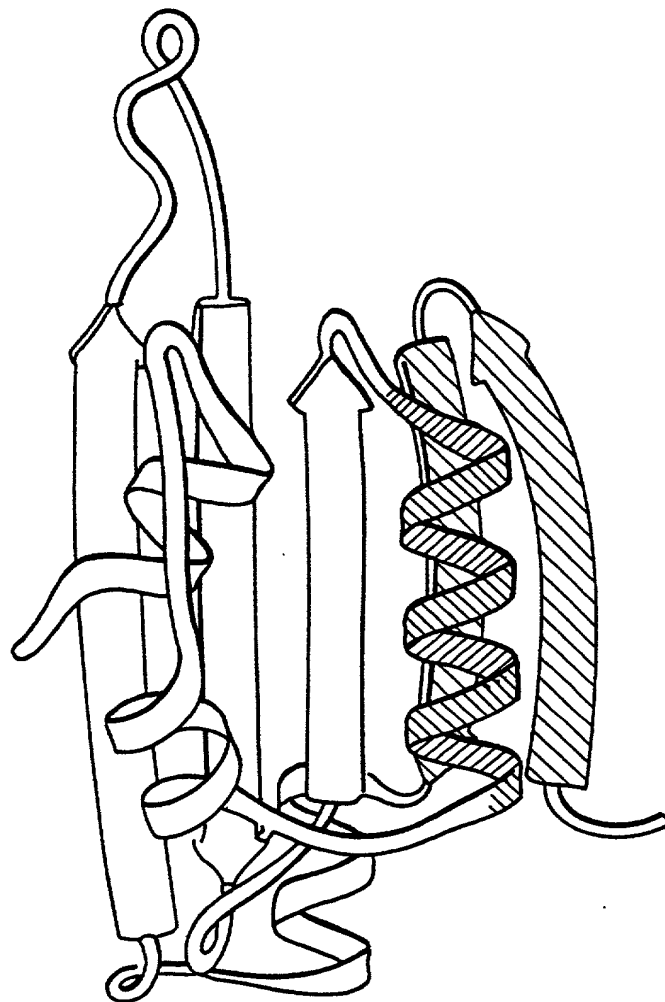


Fig. 47 A



KEY PROTEIN A

Fig. 47 B



PROTEIN B HAVING A SIMILAR STRUCTURE